

1. Research Project objectives

The overall objective of the project is to provide insight into the impact of severe plastic deformation on the microstructure and the mechanical and functional (corrosion resistance, biocompatibility) properties of the low Young modulus ($E = 60$ GPa) Ti-29Nb-13Ta-4.6Zr alloy, which belongs to a new group of Ti-based biomaterials. In addition to the general objective three special goals have been set: (i) determination of the critical deformation level required to form the nanostructure in the TNTZ alloy, (ii) analysis of the influence of grain refinement on the structure and physico-chemical properties of the surface oxide layer, and (iii) identification of the solute self-interaction mechanism responsible for the reduction in stiffness which takes place in TNTZ alloy. The hypothesis of this project is as follows: Microstructural changes which stem from severe plastic deformation improve not only mechanical properties but have also positive effect on corrosion resistance and biocompatibility of Ti-29Nb-13Ta-4.6Zr alloy.

2. Research project methodology

In order to prove the proposed hypothesis, samples with markedly different microstructures (grain size in the range from nano- to tens of micrometers) will be fabricated. Diverse grain size and deformation level will be obtained by multiple-pass cold rolling process performed on initially solution treated alloy. Microstructure characterisation will include grain size, dislocation density and phase composition measurements as well as texture investigation. The above activities allow to determine the critical deformation level needed to form the nanostructure in the studied alloy. Next, influence of large plastic deformation on: mechanical properties (hardness and tensile tests, Young modulus measurements), corrosion resistance (two corrosion environments: saline solution and artificial saliva also with fluoride ions) and biocompatibility (protein adsorption tests, surface metallic ion release and cellular investigations, including adhesion, proliferation and differentiation of osteoblasts) of TNTZ alloy will be evaluated. Physico-chemical surface properties important in the context of biocompatibility and corrosion resistance will be also studied extensively. Planned research includes: determination of chemical/phase composition and thickness of the oxide layer, measurements of contact angle and the free surface energy and finally surface topography - all studies will be executed on solution treated and cold rolled material. Experimental research will be supported by ab initio modelling of ternary and quaternary beta Ti alloys. Atomic scale mechanisms responsible for low stiffness of multicomponent Ti-based systems will be investigated through atomic bond characterisation and the binding energy calculations between Nb and a series of transition (e.g. Ta, Zr, Mo, Co, Zn) and simple (e.g. Al, Sn) metals located in a beta Ti crystal lattice.

3. Expected impact of the research project on the development of science, civilization and society

The proposed project is of high scientific importance and concerns the latest trends in materials science in the field of nano- and biomaterials. The main idea of the project is to use conventional plastic deformation methods to produce nanostructured biomaterials which allows to transfer the promising results in the laboratory to practical use. Comprehensive identification of the influence of plastic deformation on the properties of Ti-29Nb-13Ta-4.6Zr alloy is important not only for its real application, but also for future design strategy of optimal material for use in bone prosthesis. Finally, results of ab initio modelling will be highly valuable in the context of atomic-scale mechanisms responsible for the low stiffness of TNTZ alloy and will open the way to introducing a new electronic (solute interaction) parameter to aid the design of new multicomponent metastable biomedical Ti alloys.